Delicacy, Imprecision, and Uncertainty of Oceanic Simulations: An Investigation with the Regional Oceanic Modeling System (ROMS)

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LONG-TERM GOALS

In this project our long-term goal is to determine the ways and degrees to which realistically complex oceanic and atmospheric simulation models have an irreducible imprecision, hence an irreducible uncertainty in their analysis and forecast products. This goal is a natural accompaniment to the goal of continuing the evolution of the Regional Oceanic Modeling System (ROMS) as a multi-scale, multi-process model and utilizing it for studying a variety of oceanic phenomena that span a scale range from turbulence to basin-scale circulation.

OBJECTIVES

Primary objectives are code improvements and oceanographic simulation studies with ROMS, as well as with Large Eddy Simulation (LES) for boundary layer turbulence, with measurement comparisons where feasible. The targeted phenomena are submesoscale wakes, fronts, and eddies; shelf and near shore currents; internal tides; regional, Pacific and Atlantic eddy-resolving circulations and their low-frequency variability; mesoscale ocean-atmosphere coupling; and planetary boundary layers with surface gravity waves. A parallel in this project objective is to establish the characteristics of model delicacy and uncertainty in ROMS and other models for realistic simulation of highly turbulent flows, as an intrinsic model contribution to analysis and forecast errors that, in principle, is distinct from unskillful model design choices and input data errors that lead to poor solutions. The premise is that defensible alternative model designs — in parameter values, subgrid-scale parametrizations, resolution, algorithms, topography, and forcing data — may often provide a range of answers comparable to the model-measurement discrepancies. We hypothesize that some appreciable part of the model-to-measurement and model-to-model differences may be irreducibly inherent in the mathematical structure of modern simulation models.

APPROACH

The hypothesis of irreducible imprecision and uncertainty is not directly testable in any single simulation. Rather its testing is approached through a collection of simulations that examine alternative model formulations and explore the sensitivities of the answers. For a given solution feature, one can ask: Is it robust in alternative model formulations? Is it discrepant from theoretical expectations, from other model solutions, or from measurements? If so, how can the model be alternatively configured to modify these discrepancies? If the alternative model solutions cannot remove the discrepancies, then it is appropriate to conclude that either the models or the comparison standards are incorrect. If instead the solutions to alternative plausibly formulated models have a wide range of variation that encompasses the measurements and their uncertainties, then it is appropriate to conclude that there is an irreducible imprecision in the model. This approach of

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exploring all reasonable formulation alternatives with respect to all relevant solution features is essentially one of exhaustion. In practice, progress is made by the dual paths of trying to reduce the model discrepancies and educing examples of disconcertingly persistent delicacies in their answers. From this experience comes at least provisional assessments of the irreducible uncertainty.
To address these problems we are making ROMS more of a multi-process, multi-purpose, multi-scale model by including the coupling of the core circulation dynamics to surface gravity waves; sediment resuspension and transport; biogeochemistry and ecosystems; non-hydrostatic large-eddy simulation; and mesoscale atmospheric circulation, and by providing a framework for data-assimilation analyses (led by others). In addition we continue to refine the core algorithms, for which evidence of solution delicacy is an excellent guide for where improvements may be helpful. Furthermore, to expand the range of model solutions used to test model sensitivities through collaborations, we also use Large Eddy Simulation for the atmospheric and oceanic surface boundary layers (with Peter Sullivan, NCAR), the ITCP atmospheric general circulation model (with Annalisa Bracco, Georgia Tech), and an intermediate-complexity model of El Niño – Southern Oscillation, ENSO (with Mickael Chekroun and David Neelin, UCLA).

WORK COMPLETED

In the past year we have worked on the following circulation regimes and phenomena: decadal Pacific and Atlantic circulations; equilibrium regional circulations in the U.S. West Coast, central Alaska, Central and South America, Solomon Sea, the Kuroshio, and the Gulf Stream; mesoscale eddy buoyancy fluxes; submesoscale surface fronts, filaments, and eddies; topographic current separation, form stress, and submesoscale vortex generation; surface waves and nearshore currents and internal tides in Southern California; surface wave influences on the turbulent boundary layer and littoral currents; bubbles generated by wave breaking; mesoscale air-sea coupling using ROMS and WRF; the atmospheric general circulation using the ITCP AGCM; and the intermediate ENSO model. The ROMS algorithmic work has been on adapting the oceanic equation of state for split-explicit time stepping of barotropic and baroclinic modes; accurate time-stepping for the bottom boundary layer in shallow water ($\sim$ meters) and wake flows past topography; open boundary conditions for highly turbulent flows; incorporating surface wave effects in ROMS; diagnosing spurious diapycnal mixing due to advection errors and designing remedies; a new model of a size-distributed bubble population; and the exploration of several test-bed configurations for the simulation delicacy investigation.

RESULTS

We present a few highlights for this project. The publications list (papers from 2012 up to ones likely to be submitted in 2013) provides a view of the finalized results across all our ONR projects.

Decision Dilemmas in Parameter Choices: An important source of uncertainty in ocean and climate models is linked to the calibration of model parameters. Interest in systematic and automated parameter optimization procedures stems from the desire to improve the model climatology and to quantify the average sensitivity associated with potential changes in the climate system. Building upon the smoothness of the response of low-order statistical measures of the discrepancy from observations in an atmospheric circulation model (AGCM) to changes of four adjustable parameters, Neelin *et al.* (*PNAS*, 2010) used a quadratic metamodel to objectively calibrate the International Centre for Theoretical Physics (ICTP) AGCM. The metamodel accurately estimates global spatial averages of common fields of climatic interest, from precipitation, to low and high level winds, from temperature at various levels to sea level pressure and geopotential height, while providing a computationally cheap strategy to explore the influence of parameter settings. Here, guided by the metamodel, the ambiguities or dilemmas related to the decision making process in relation to model

sensitivity and optimization are examined. Global simulations of current climate are subject to considerable regional-scale biases. Those biases may vary substantially depending on the climate variable considered, and/or on the performance metric adopted. Common dilemmas are associated with model revisions yielding improvement in one field or regional pattern or season, but degradation in another, or improvement in the model climatology but degradation in the interannual variability representation. Challenges are posed to the modeler by the high dimensionality of the model output fields and by the large number of adjustable parameters. The use of the metamodel in the optimization strategy helps visualize trade-offs at a regional level, *e.g.,* how mismatches between sensitivity and error spatial fields yield regional errors under minimization of global objective functions. The implication of this analysis is that, at least with a modern AGCM, the attempt to optimally choose model parameters to reduce its errors with observations encounters severe regional conflicts between improvements for some places and quantities at the cost of degradation in others. Pending the creation of a more accurate model, the modeler is left with unresolvable dilemmas in the best choice of model parameters, which is a type of irreducible uncertainty (Bracco *et al.*, 2013).

Rough Parameter Dependences: Despite the importance of uncertainties encountered in ocean and climate model simulations, the fundamental mechanisms at the origin of sensitive behavior of long-term model statistics remain unclear. Variability of turbulent flows in the atmosphere and ocean exhibits recurrent large-scale patterns. These patterns, while evolving irregularly in time, manifest characteristic frequencies across a large range of time scales, from intraseasonal through interdecadal. Based on modern spectral theory of chaotic and dissipative dynamical systems, the associated low-frequency variability (LFV) may be formulated in terms of Ruelle-Pollicott (RP) resonances. RP resonances encode information on the nonlinear dynamics of the system, and a natural approach for estimating them — as filtered through an "observable" (output variable) of the system — is proposed. This approach relies on an appropriate Markov representation of the dynamics associated with a given observable. It is shown that, within this representation, the spectral gap — defined as the distance between the subdominant RP resonance and the unit circle — plays a major role in the roughness of the parameter dependence. The model statistics are the most sensitive for the smallest spectral gaps; such small gaps turn out to correspond to regimes where the LFV is more pronounced, while autocorrelations decay more slowly. This approach is applied to analyze the rough parameter dependence encountered in key statistics of an El Niño - Southern Oscillation model of intermediate complexity (originally due to Jin & Neelin, *JAS*, 1993). It shows that in parameter regimes with greater amplitude for the spontaneous LFV, model statistics for some output variables are more sensitive to small changes in the model parameters than they are in regimes with lesser LFV (Fig. 1; Chekroun *et al.*, 2013). Because the values for model parameters will never be known with high precision, a highly rough parameter dependency of model solutions represents an irreducible uncertainty. Theoretical arguments strongly suggest that such links between model parameter sensitivity and the decay of correlation properties are not limited to this particular model and could hold much more generally. However, it may be much more subtle to identify the appropriate observables that display this behavior in a fully realistic general circulation model.

Circulation Delicacy due to Wind and Topography: Widespread experience in basin-scale oceanic modeling indicates a high degree of sensitivity of strong currents to many aspects of the simulation configuration, especially for western boundary currents and their pathway following boundary separation. We are exploring the influences of the wind forcing and domain configuration. Following the approach described in Lemarie *et al.* (2012a), we have decadal, basin-scale ROMS solutions for the Pacific Ocean at a horizontal grid resolution of $dx = 12.5$ km and other solutions for the Atlantic Ocean with $dx = 7$ km. For each of these a number of sensitivity experiments have been performed

with variations in the wind forcing and the domain shape and topography; we restrict ourselves to only plausibly realistic variations, *i.e.,* ones justified by different data sets with alternative interpolation and smoothing procedures to adapt to the model grid. In previous annual reports we described remote sensitivities to changes in the wind and topography far away from the separating boundary current. Another example is a local topographic sensitivity for the Kuroshio Current as it flows north past Luzon Strait between Taiwan and the Philippines. While observations show that there are occasional westward loop intrusions of the Kuroshio into the Strait, the pair of solutions in Fig. 2 show a much more extreme sensitivity than is observed. Motivated by results in Metzger & Hurlbert (*GRL*, 2001), several islands that were not automatically resolved by the model grid were manually added to the land mask. By this alteration in the representation of small islands in the Strait, the modeled time-averaged Kuroshio can either cross the Strait or penetrate deeply westward into the South China Sea. The latter configuration would be rejected by a modeler on the basis of its embarrassing solution. Nevertheless, the topographic representation involves somewhat arbitrary and *ad hoc* decisions about whether to include particular small islands and how to smooth the bathymetric data at a given model resolution. Within a less extreme range of model results, there may be no physically principled way of eliminating this type of sensitivity apart from further increasing the grid resolution (which may just move the sensitivity to currents on smaller scales). *Post hoc* selection of the topographic representation based on a particular solution feature, here the Kuroshio path, would be an unprincipled choice that is likely to increase errors in other features (*cf.,* the "decision dilemma" above). We are currently working on manuscripts that report the experiences with wind and topographic sensitivities for western boundary currents, as well as describe good algorithmic practices for the data handling for the model grid.

Treatment of oceanic topography: While it is universally accepted that bottom topography plays a major controlling role over oceanic flows, the practices associated with handling topography in oceanic models are far from settled at the present time. The issues are three-fold: (*i*) uncertainties (and in some cases contradictions) associated with available data sets; (*ii*) procedures associated with preparation of topography for numerical oceanic modeling; (*iii*) topographic sensitivity of numerical algorithms within the oceanic modeling codes.

The first one, (*i*), is illustrated by Fig. 3. We plotted topography from eight different datasets in an identical format using logarithmic scaling to highlight contours in shallow areas. At first, it is quite striking that consecutive versions of datasets coming from the same source may be radically different without an obvious tendency to converge. There is also unexpected historical commonality between some versions taken from the different sources. Superficially, paying attention to the features between Taiwan and Mainland China, the datasets can be categorized into three groups: SRTM30 (Jan. 2013), GEBCO_08 (Sept. 2010), and ETOPO1 (Jan. 2013) show a channel-like deeper passage winding toward Mainland and then going along the coast; ETOPO2v2c_f4,2006 and GEBCO 1min, 2008 show shallow bank protruding from Taiwan toward China (it is somewhat present in ETOPO1, Jan. 2013 as well). In our practical experience we found that topography from this group tends to generate "hot spots" (specific places that impose a numerical restriction to maintain stability) between China and Taiwan; ETOPO2v.1, 2001 and SRTM30, 2011 just show a rough irregular pattern in the same area. Finally, we note that even the most modern datasets [GEBCO_08, Sept. 2010, SRTM30, Jan. 2013, and ETOPO1, Jan. 2013] still contain significant differences (up to 500m in depth values of depth), and in features, which cannot be explained by differences in interpolation and data quality control.

The second one, (*ii*), is associated with the fact that in today's ocean modeling practice topographic datasets are available at resolutions which are typically higher than model grids. This means that the data must be essentially coarsened, which unavoidably leads to suppression of some topographic

features. The mathematical optimization dilemma of how to keep model topography representative of the realistic one, but at the same time numerically acceptable by the modeling code, is not uniquely solvable. For example, smoothing of a ridge while conserving its volume unavoidably leads to the reduction of its height, which changes the regime by opening a path which should not be open. On the other hand, maintaining the height, while reducing the steepness of the slopes leads to an increase of volume, which still may be preferred. It is not surprising that historical publications related to this subject (*e.g.,* Mellor *et al.*, *JAOT*, 1994; Martinho & Batteen, *OM*, 2006; Sikirić *et al.*, *OM*, 2009) advocate very different criteria. We have developed robust techniques for transferring data topography into model grid (including both averaging/dealiasing, and enforcing numerical slope constraints); however, the main criterion of success remains the behavior of modeled flow as the result of simulation, rater than satisfying an *a priori* selected constraint. This leaves a degree of empiricism and an unavoidable imprecision. Figure 4 illustrates sensitivity of the flow regime to topographic slope in a superficially simple case of barotropic flow past and obstacle – a cylindrical island. The slope is rather gentle and there are no numerical concerns about the accuracy of this simulation. Yet, the flow regime changes in an unintuitive way with a smoothly changing controlling parameter. When the slope is weak (bottom panel), the pattern is similar to a vortex street with cyclonic and anticyclonic eddies alternately shed from the left and right side of the island. Once the slope reaches a certain value (0.34% to 0.38%), no eddies are shed, and the wake only oscillates slightly around the midline. Further increase of the slope leads to a highly non-stationary regime again. While the mechanism of such change cannot be fully explained, we note that increase of the slope results in proportional increase of the speed of topographic Rossby waves, which at some point match the inflow velocity (in this configuration Rossby waves propagate upstream) resulting in qualitatively distinct *below*, *match*, and *above* regimes, while no further qualitative changes are expected outside this range of parameters (experiments with opposite-sign slope reveal no special behavior).

Code algorithmic sensitivity to topography, item (*iii*), is a widely known topic (*e.g.,* sigma-coordinate pressure-gradient errors, spurious mixing), yet some of its aspects are much less noted. Theoretical studies of the stability of barotropic-baroclinic mode splitting stay entirely within the consideration of linear internal and external waves in layered systems over a flat bottom (Higdon & Bennett, *JCP*, 1996, *et seq.*). Practical oceanic modeling requires nonlinear advection, topography, and mode splitting. Figure 5 shows a numerical instability associated with improper computation of advection terms due to splitting. In principle, this type of instability occurs even without topography, but with topography it was first pointed out by Morel *et al.* (*OM*, 2008) in the context of HYCOM (they propose a remedy), but in fact, this would occur in every existing modeling code that does not recompute advection terms within the barotropic mode (*e.g.,* MOM, POP, *etc.*). Originally ROMS and POM do so (hence are not subject to such instability), however this clearly comes with extra computational cost, so we have redesigned the code for efficiency, while having an approach different from that of Morel *et al.* (2008).

IMPACT/APPLICATIONS

Geochemistry and Ecosystems: An important community use for ROMS is biogeochemisty: chemical cycles, water quality, blooms, micro-nutrients, larval dispersal, biome transitions, and coupling to higher tropic levels. We collaborate with Profs. Keith Stolzenbach (UCLA), Curtis Deutsch (UCLA), David Siegel (UCSB), and Yusuke Uchiyama (Kobe).

Data Assimilation: We collaborate with Drs. Zhinjin Li (JPL), Yi Chao (Remote Sensing Solutions), and Kayo Ide (U. Maryland) by developing model configurations for targeted regions and by consulting on the data-assimilation system design and performance. Current quasi-operational, 3DVar applications are in California (SCCOOS and CenCOOS) and in Alaska (Prince William Sound).

TRANSITIONS

ROMS is a community code with widespread applications (http://www.myroms.org).

RELATED PROJECTS

Three Integrated Ocean Observing System (IOOS) regional projects for California and Alaska (SCCOOS, CenCOOS, and AOOS) utilize ROMS for data assimilation analyses and forecasts.

PUBLICATIONS

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FIGURES

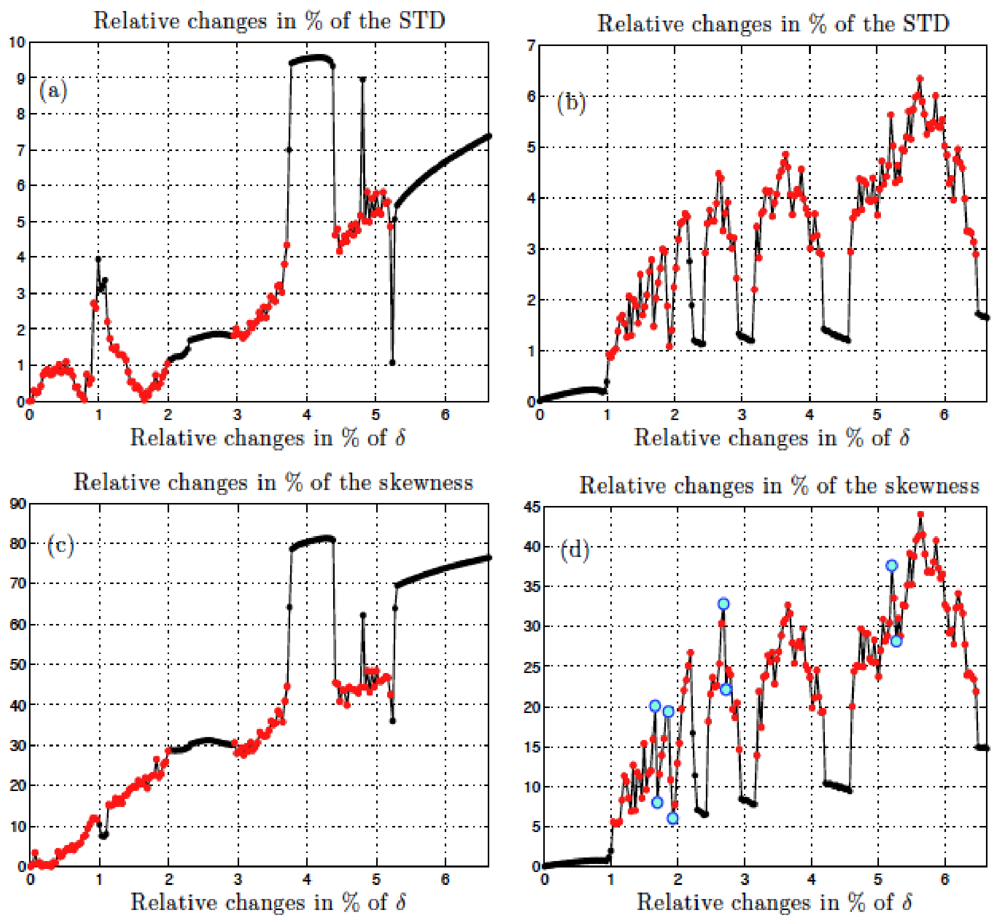


Figure 1: ***Statistical sensitivity of the Niño-3 SST "observable" in an intermediate complexity model of El Niño - Southern Oscillation. Plotted are relative changes in percentage for the standard deviation (STD) and skewness with respect to variations in δ, a parameter affecting the trans-Pacific travel time of equatorial ocean waves. Panels (a) and (c) correspond to a model parameter-set that yields a "rapidly mixing" regime with little low-frequency variability (LFV), and they show relatively smooth variations with δ except for a few bifurcation points. Panels (b) and (d) correspond to a "slowly mixing" regime with more LFV. In each of these panels, the chaotic (resp. periodic or quasi-periodic) behavior is represented by red (resp. black) dots. In panel (d), two consecutive cyan dots represent local changes in the skewness from about 9.5 % to 13.5 %, for corresponding variations in δ of less than 0.06 %. (Chekroun*** et al.***, 2013).***

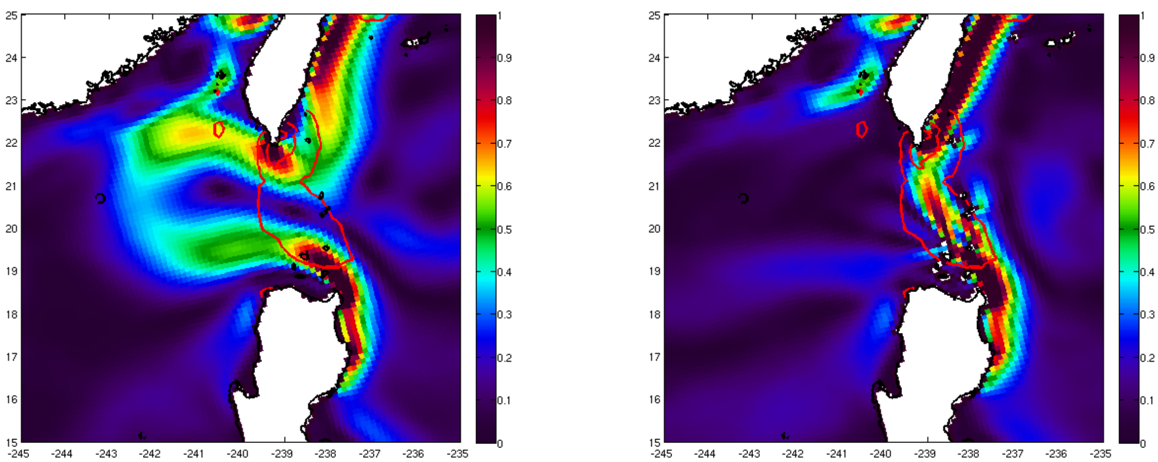
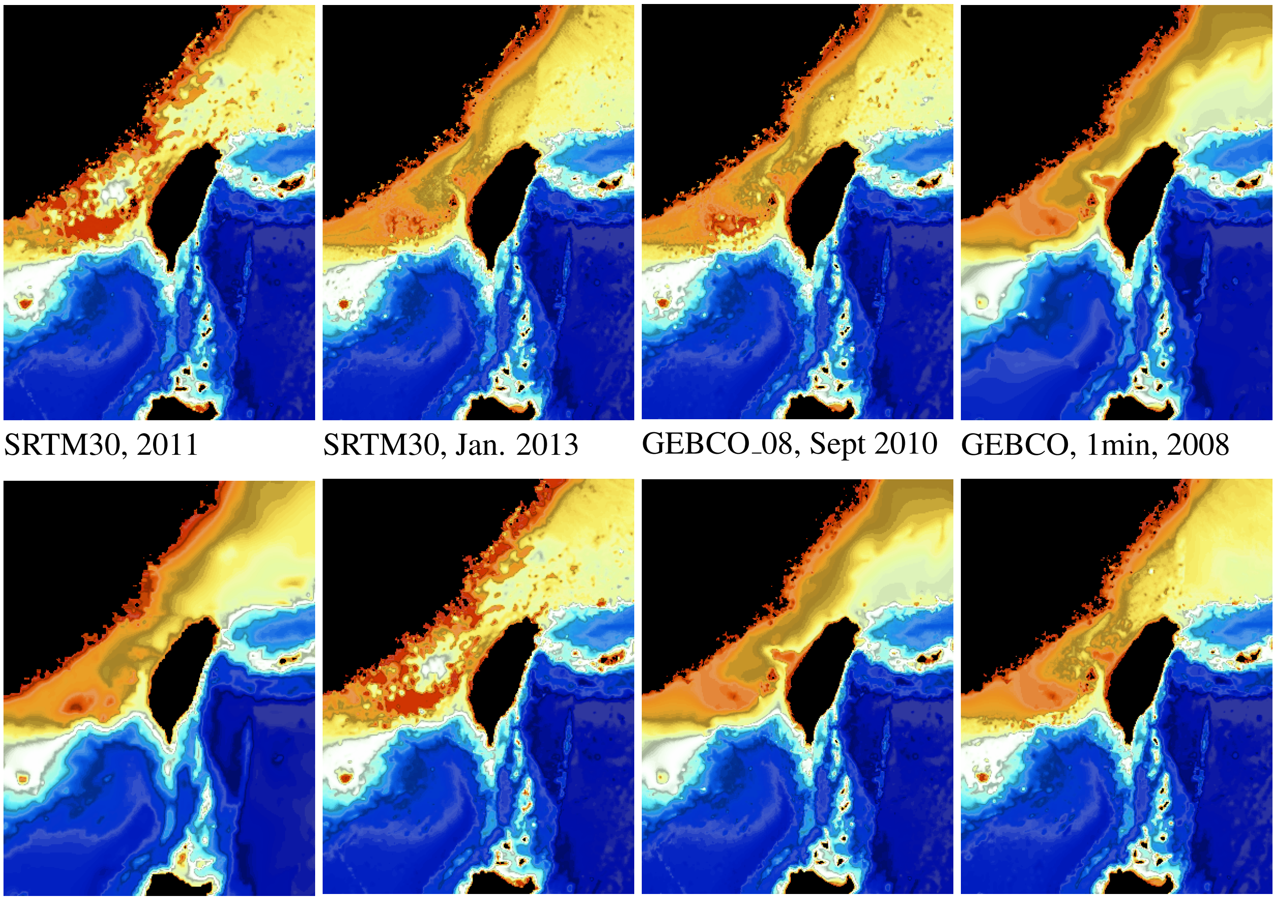


Figure 2: ***Annual mean sea-surface geostrophic current speed [m s^{-1}] near the Luzon strait in the Western North Pacific Ocean. Indicated with a red solid line is the*** $0.3\ m/s$ ***contour level from the AVISO altimetry data set. Left and right panels differ only in the land mask for islands at four grid points inside the Luzon strait. Local changes in the solution are extremely large. In one case the correspondence with AVISO is rather good, and in the other it is very poor. Similar topographic sensitivity in this region is reported in Hurlburt & Metzger (*GRL*, 2001) for a different model.***



SRTM30, 2011 | SRTM30, Jan. 2013 | GEBCO_08, Sept 2010 | GEBCO, 1min, 2008

ETOPO5 | ETOPO2 v.1, 2001 | ETOPO2v2c_f4, 2006 | ETOPO1, Jan 2013

Figure 3: ***Comparison of bottom topography data from eight datasets used in ocean modeling for the area of Taiwan andthe Luzon Strait.***

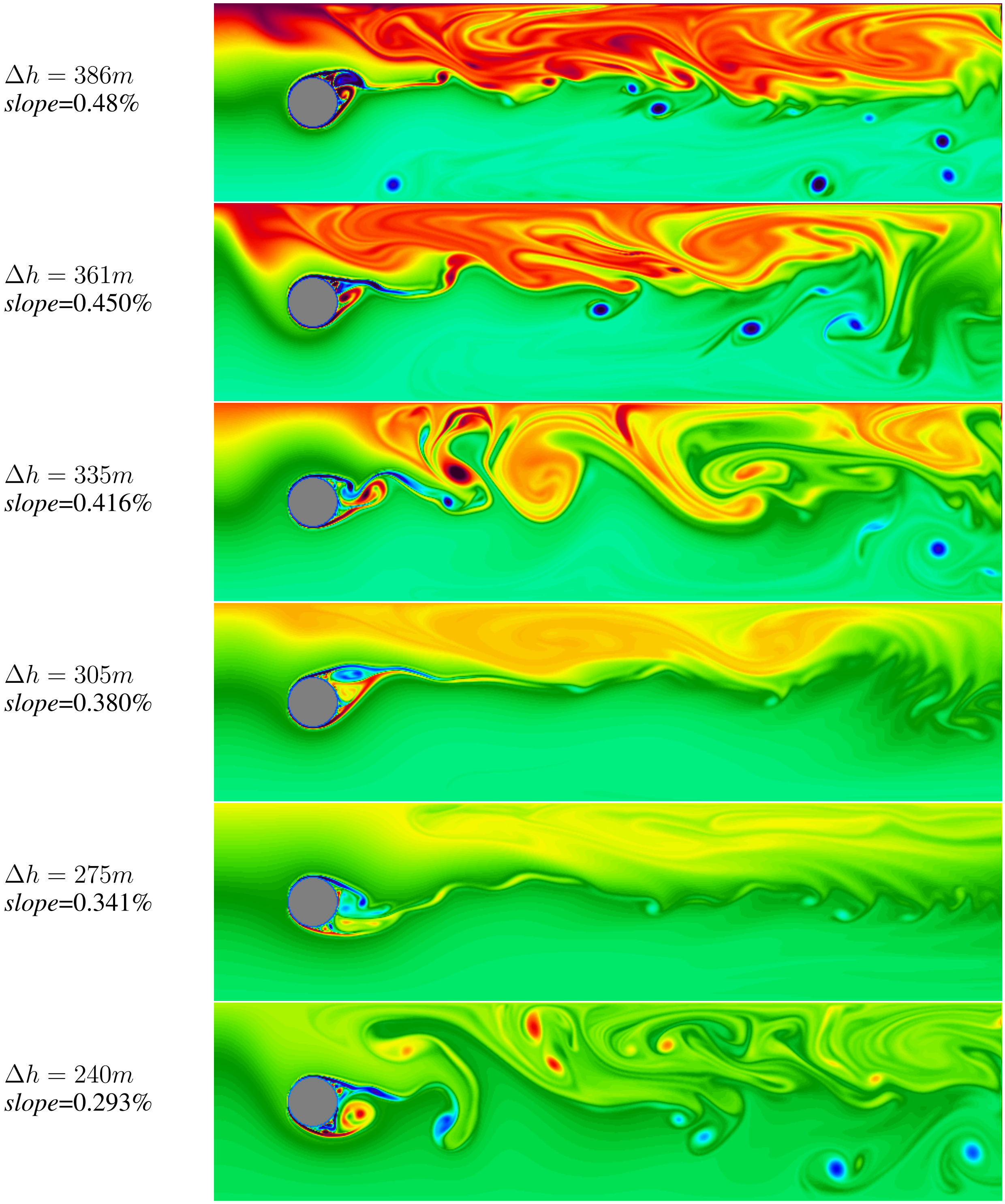


Figure 4: ***An example of topographic sensitivity of flow regime in an idealized barotropic island wake over sloping bottom. Field shown is barotropic potential vorticity,*** $BPV = \dfrac{f + \nabla \times \overline{\mathbf{u}}}{h + \zeta}$***. The domain is 320 km long and 80 km wide with a circular island of 20 km in diameter, channel configuration. The inflow velocity is 0.15 m s***$^{-1}$***, uniform in horizontal and vertical directions, and the Coriolis parameter is*** $f = 10^{-4}$ ***s***$^{-1}$***. In all the cases the depth is*** h***=500m at the southern side of the domain, and it reduces toward the north reaching*** $h - \Delta h$ ***at the northern side, with*** Δh ***specified on the left in each panel. Also specified is the absolute slope,*** $\partial h/\partial y$***, expressed in %.***

$\Delta t = 60sec$
$M = 17$

$\Delta t = 120sec$
$M = 33$

$\Delta t = 180sec$
$M = 50$

$\Delta t = 200sec$
$M = 55$

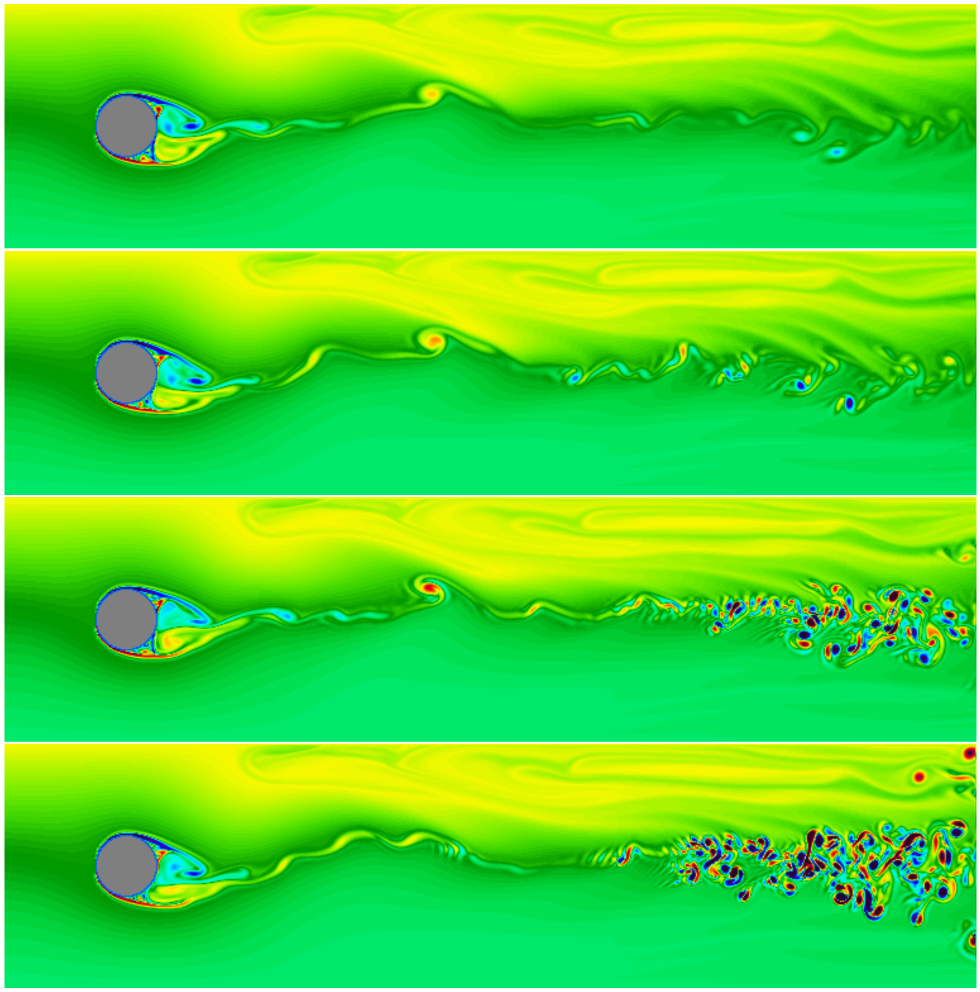


Figure 5: ***An example of weak numerical instability caused by inaccurate mode splitting. All the conditions are the same as in Fig. 4, the second panel from the bottom, $\Delta h = 275m$, except that in this simulation vertically averaged velocity components participating in computation of r.h.s. terms for 3D momentum equations are time centered at nth step (not extrapolated to $n + 1/2$), and there is also no recomputing of advective terms at at every time step within the barotropic mode. Δt indicated on the left of each panel is the time step for 3D mode, and M is the mode splitting ratio (the barotropic time step $\Delta t/M$ is approximately the same for each panel). Notice a non-physical instability of the wake, which is strongly dependent on the size of the time step. Consistent mode splitting (either extrapolated vertical averages or recomputed barotropic advective terms) do not exhibit such sensitivity.***